# Metropolis Monte Carlo algorithm based on reparametrization invariance

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## Abstract

We introduce a modification of the well-known Metropolis importance sampling algorithm by using a methodology inspired on the consideration of the *reparametrization invariance* of the microcanonical ensemble. The most important feature of the present proposal is the possibility of performing a suitable description of microcanonical thermodynamic states during the first-order phase transitions by using this local Monte Carlo algorithm.

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## I. INTRODUCTION

The basic problem in equilibrium statistical mechanics is to compute the phase space average, in which Monte Carlo method plays a very important role [1, 2, 3]. Among all admissible statistical ensembles used with the above purpose, the microcanonical ensemble provides the most complete characterization of a given system in thermodynamic equilibrium. While microcanonical calculations based on microscopic dynamics can suffer from the existence of metastable states with large relaxation times [4, 5], the available Monte Carlo methods based on reweighting technics (such as the Multicanonical Monte Carlo [6, 7]) are also so much machine-time consuming due to they try to obtain the density of states for all values of energy in only one run. It is very well known that the microcanonical observables can be suitably obtained by using the canonical ensemble whenever *ensemble equivalence* takes place in a sufficient large system.

One of the most famous and widely used Monte Carlo algorithm considering the Gibbs canonical ensemble is the Metropolis importance sampling algorithm [8]. This method has some important features. It is extremely general and each moves involves $O(1)$ operations. However, its dynamics suffers from *critical slowing down,* that is, if $N$ is the system size, the correlation time $\tau$ diverges as a critical temperature is approached: the divergence follows a power law behavior $\tau \propto N^z$ in second-order phase transitions, while $\tau$ diverges exponentially with $N$ in first-order phase transitions as consequence of the ensemble inequivalence (multimodal character of the energy distribution function).

The aim of the present Letter is to develop a new methodology in which the local algorithm Metropolis Monte Carlo could be used for performing microcanonical calculations by avoiding the anomalous behaviors associated with the presence of a first order phase transition in a given energetic region. The key of our method is to consider certain generalized canonical-like ensemble which is equivalent to the microcanonical ensemble for $N$ large enough in spite of the presence of a first-order phase transition, a methodology inspired by our recent paper [9].

## II. THE METHOD

Let us consider a given Hamiltonian system $\hat{H}$ becoming extensive in the thermodynamic limit $N \to \infty$. As already commented, the basic idea of our method is to substitute the Gibbs canonical ensemble by the following *generalized canonical ensemble*:

$$\hat{\omega}_c(\eta, N) = \frac{1}{Z_c(\eta, N)} \exp\left(-\eta \Theta\left(\hat{H}\right)\right), \tag{1}$$

where $\Theta(E) \equiv N\varphi(E/N)$, being $\varphi(\varepsilon)$ certain analytical *bijective function* of the energy per particle of the system $\varepsilon = E/N$.

The *Planck potential* $\mathcal{P}(\eta, N) = -\ln Z_c(\eta, N)$ associated with the partition function:

$$Z_c(\eta, N) = \int \exp\left(-\eta N \varphi\left(\frac{1}{N}E\right)\right) \Omega(E, N)\, dE, \tag{2}$$

can be estimated for $N$ large by using the steepest descend method as follows:

$$\mathcal{P}(\eta, N) \simeq N\{\eta\varphi(\varepsilon_e) - s(\varepsilon_e)\} - \frac{1}{2}\ln\left(\frac{2\pi\sigma_\varepsilon^2(\varepsilon_e)}{N}\right), \tag{3}$$

where $s(\varepsilon) = \ln\langle W(E, N)\rangle / N$ is the entropy per particle of the system, being $W = \Omega(E, N)\,\delta\varepsilon_0$ the microcanonical accessible volume, and $\varepsilon_e$, the *only one* stationary energy of the maximization problem $\max_{\varepsilon_e}\{\eta\varphi(\varepsilon) - s(\varepsilon)\}$ whose stationary conditions demand:

$$\eta\frac{\partial\varphi(\varepsilon_e)}{\partial\varepsilon} = \frac{\partial s(\varepsilon_e)}{\partial\varepsilon} \text{ and} \tag{4}$$

$$\frac{1}{\sigma_\varepsilon^2(\varepsilon_e)} = \eta\frac{\partial^2\varphi(\varepsilon_e)}{\partial\varepsilon^2} - \frac{\partial^2 s(\varepsilon_e)}{\partial\varepsilon^2} > 0. \tag{5}$$

We found by combining (4) and (5) that the necessary and sufficient condition for the existence of a unique stationary point of the above maximization problem for any $\eta$ is given by:

$$-\frac{\partial\varphi(\varepsilon)}{\partial\varepsilon}\frac{\partial}{\partial\varepsilon}\left\{\left(\frac{\partial\varphi(\varepsilon)}{\partial\varepsilon}\right)^{-1}\frac{\partial s(\varepsilon)}{\partial\varepsilon}\right\} > 0, \tag{6}$$

which has to be applicable for all those admissible values of the energy per particle $\varepsilon$. This condition can be rephrased by considering the inverse function $\varepsilon(\varphi)$ of the bijective function $\varphi(\varepsilon)$, and taking the entropy $s$ as a *scalar function* which is now rewritten in terms of the variable $\varphi$:

$$s(\varphi) \equiv s[\varepsilon(\varphi)] \Rightarrow -\left(\frac{\partial\varphi(\varepsilon)}{\partial\varepsilon}\right)^2 \frac{\partial^2 s(\varphi)}{\partial\varphi^2} > 0, \qquad (7)$$

which clarifies us that the entropy must be a concave function in this last parametrization.

The approximation (3) in the thermodynamic limit is just the Legendre transformation between the thermodynamic potentials, $\mathcal{P}(\eta, N) \simeq \eta\Theta - S(\Theta, N)$ with $S(\Theta, N) = S(E, N)$, which takes place as a consequence of the equivalence between the generalized canonical ensemble (1) and the microcanonical ensemble. Thus, *we can ensure the ensemble equivalence for all energy values by using an appropriate bijective function $\varphi(\varepsilon)$ without mattering about the presence of a first-order phase transition.* This remark is precisely the key of the Metropolis algorithm described below.

Considering the analogy with the Gibbs canonical ensemble, the generalized canonical ensemble represents a system in which the parameter $\eta$ associated with the macroscopic observable $\Theta$ is keeping fixed by means of certain external experimental arrangement. The state above is just a consequence of the reparametrization invariance of the microcanonical ensemble: the microcanonical description does not depend on the reparametrization $\Theta = N\varphi(E/N)$ used for describing the equilibrium thermodynamical states of the system. We only discuss in the present work the applicability of this symmetry in improving the ordinary Metropolis importance sampling algorithm based on the Gibbs canonical ensemble (hereafter MMC), but the interested reader can see the recent paper [9] about the implication of the reparametrization invariance in the searching of a topological classification scheme of the phase transitions.

Generally speaking, the main difference between the MMC and the Metropolis algorithm based on the reparametrization invariance (hereafter GCMMC) is the using of the canonical-like weight $\omega(E) = \exp(-\eta\Theta(E))$. Therefore, the probability $p$ for the acceptance of a Metropolis move is given by:

$$\begin{aligned} p &= \min\{1, \exp\{-\eta[\Theta(E+\Delta\varepsilon) - \Theta(E)]\}\} \\ &\simeq \min\left\{1, \exp\left[-\eta\frac{\partial\varphi(\varepsilon)}{\partial\varepsilon}\Delta\varepsilon - \frac{1}{2N}\eta\frac{\partial^2\varphi(\varepsilon)}{\partial\varepsilon^2}\Delta\varepsilon^2\right]\right\}, \end{aligned} \qquad (8)$$

in which all $O\left(\frac{1}{N}\right)$ contributions in the exponential argument have been dismissed. While every energy decreasing $\Delta\varepsilon < 0$ is always accepted in the MMC, such probability decreases in the GCMMC due to the presence of the quadratic term in the exponential argument of (8), although such effect decreases with the $N$ increasing.

Obviously, when $N$ is large enough, the expression of the acceptance probability of the GCMMC differs effectively from the one used in the MMC by the consideration of a *variable canonical parameter* $\beta(\varepsilon; \eta)$:

$$\beta(\varepsilon; \eta) = \eta\frac{\partial\varphi(\varepsilon)}{\partial\varepsilon}, \qquad (9)$$

which fluctuates around the microcanonical value $\beta(\varepsilon_e) = \partial s(\varepsilon_e)/\partial\varepsilon$ derived from the condition (4). Taking into account the sharp Gaussian localization of the integral (2) in the thermodynamic limit, the dispersion $\delta\beta \equiv \sqrt{\langle\delta\beta^2\rangle}$ can be estimated in terms of the energy dispersion $\delta\varepsilon \equiv \sqrt{\langle\delta\varepsilon^2\rangle}$ as follows:

$$\delta\beta = \eta\frac{\partial^2\varphi(\varepsilon_e)}{\partial\varepsilon^2}\delta\varepsilon, \qquad (10)$$

where $\langle\cdots\rangle$ denotes the average over the ensemble (1). Considering the Gaussian estimation of the energy dispersion as $\langle\delta\varepsilon^2\rangle = \sigma_\varepsilon^2(\varepsilon_e)/N$ with $\sigma_\varepsilon^2(\varepsilon_e)$ given in (5), the equation (10) can be rewritten in the following form:

$$\delta\beta = \frac{1}{N\delta\varepsilon} + \delta\varepsilon\frac{\partial^2 s(\varepsilon)}{\partial\varepsilon^2}. \qquad (11)$$

This expression is a very nice result which talks about the limits of precision in a general calculation of the caloric curve by using a local algorithm based on the generalized canonical ensemble (1): while temperature can be fixed ($\delta\beta = 0$) wherever the entropy is a concave function, the inverse temperature dispersion $\delta\beta$ can not vanish wherever the entropy be a convex function in terms of energy $\varepsilon$. Supercritical slowing down associated with the MMC method based on the Gibbs canonical ensemble is precisely related with the downfall of the Gaussian estimation of the energy dispersion $\delta\varepsilon = \left(-N\partial^2 s(\varepsilon)/\partial\varepsilon^2\right)^{-\frac{1}{2}}$ whenever the second derivative of the entropy goes to zero and becomes nonnegative. It is very interesting to notice that the complementary macroscopic observables energy and temperature obey the *uncertainly relation* $\delta E\delta\beta \geq 1$ wherever $\partial^2 S(E, N)/\partial E^2 \geq 0$, which is rather analogue to the Quantum Mechanics uncertainly relation $\delta E\delta\tau \sim \hbar$. A better analysis allows us to obtain the inequalities $\delta\varepsilon \leq \left(-N\partial^2 s(\varepsilon)/\partial\varepsilon^2\right)^{-\frac{1}{2}}$ whenever entropy $s(\varepsilon)$ be a concave function, while $\delta\beta \geq \left(\partial^2 s(\varepsilon)/\partial\varepsilon^2/N\right)^{\frac{1}{2}}$ when entropy is convex.

As already commented, the success of the GCMMC methods relies on the selection of a good bijective function $\varphi(\varepsilon)$ satisfying the condition (7), which obviously can be done by following different schemes. For example, we can rephrase the stationary condition (4) as $\eta = \partial s(\varphi)/\partial\varphi$ and substitute it in (7). The resulting equation expresses the monotonic decreasing of the dependence $\eta$ *versus* the energy per particle $\varepsilon$:

$$\frac{\partial\eta(\varepsilon)}{\partial\varepsilon} < 0, \qquad (12)$$

which talks about a bijective correspondence between $\eta$ and $\varepsilon$ as a consequence of the ensemble equivalence. This last demand suggests us the implementation of an indirect Monte Carlo method based on the generalized canonical ensemble (1) where an arbitrary dependence $\eta(\varepsilon)$ satisfying the above condition be assumed *a priory*, but the unknown associated bijective function $\varphi(\varepsilon)$ must be reconstructed by using reweighting schemes analogue to the ones used in the Multicanonical calculations [6, 7]. Nevertheless, we are interested in the present work in the implementation of a variant of the Metropolis algorithm with acceptance probability (8) where the bijective function $\varphi(\varepsilon)$ will be proposed *a priory* in order to avoids the ensemble inequivalence in a Hamiltonian system with short-range interactions.

Let us assume that the interest system exhibits an ensemble inequivalence inside the energy interval $(\varepsilon_1, \varepsilon_2)$, where $\partial^2 s(\varepsilon_i)/\partial\varepsilon^2 < 0$. The microcanonical parameter $\beta(\varepsilon) = \partial s(\varepsilon)/\partial\varepsilon$ will change slowly with the energy $\varepsilon$ in this region due to $\left|\partial^2 s(\varepsilon)/\partial\varepsilon^2\right| \simeq 0$ in the first-order phase transitions (see in the application example described in the next section), so that, $\eta(\varepsilon)\,\partial\varphi(\varepsilon)/\partial\varepsilon \simeq \beta_c$ where $\beta_c$ is the inverse critical temperature. Assuming this last relation as a first approximation, its substitution in the condition of the ensemble equivalence (5) yields:

$$\frac{\partial\varphi(\varepsilon)}{\partial\varepsilon} = \frac{\beta_c}{\eta(\varepsilon)} \Rightarrow \frac{1}{\sigma_\varepsilon^2(\varepsilon)} \simeq \beta_c\lambda(\varepsilon) - \frac{\partial^2 s(\varepsilon)}{\partial\varepsilon^2} > 0, \quad (13)$$

with $\lambda(\varepsilon) = -\partial \ln \eta(\varepsilon)/\partial\varepsilon$. This demands is very easy to satisfy by considering the function $\lambda(\varepsilon)$ as a large enough positive constant, $\lambda(\varepsilon) \equiv \lambda > 0$. This assumption allows us to propose the first derivative of the bijective function $\varphi(\varepsilon)$ as follows:

$$\xi(\varepsilon) = \frac{\partial\varphi(\varepsilon)}{\partial\varepsilon} = \begin{cases} 1 & \text{if } \langle\varepsilon\rangle > \varepsilon_2, \\ \exp\left(-\lambda(\varepsilon_2 - \varepsilon)\right) & \text{if } \langle\varepsilon\rangle \in (\varepsilon_1, \varepsilon_2), \\ \exp\left(-\lambda(\varepsilon_2 - \varepsilon_1)\right) & \text{otherwise,} \end{cases} \quad (14)$$

which should avoid the ensemble inequivalence within the energetic range $(\varepsilon_1, \varepsilon_2)$. Since $\xi(\varepsilon)$ is a constant when $\langle\varepsilon\rangle > \varepsilon_2$ or $\langle\varepsilon\rangle < \varepsilon_1$, the GCMMC becomes in the MMC algorithm outside the interval $(\varepsilon_1, \varepsilon_2)$.

Although the piecewise function $\xi(\varepsilon)$ is referred in terms of the instantaneous values of the energy $\varepsilon$ in the Metropolis dynamics, we propose in (14) that the selection of the interval during the whole computation of the microcanonical averages at a given energy depends on the average energy $\langle\varepsilon\rangle$ instead of the instantaneous values $\varepsilon$. It can be numerically checked that the existence of any abrupt change in the first derivatives of the function $\xi(\varepsilon)$ in the acceptance probability (8) can provoke a significant perturbation in the convergence of the second derivative of the entropy (associated with the heat capacity) by using the GCMMC when the instantaneous energy $\varepsilon$ is close to $\varepsilon_1$ or $\varepsilon_2$. However, the using of $\langle\varepsilon\rangle$ instead of the instantaneous value $\varepsilon$ allows the function $\xi(\varepsilon)$ to exhibit a smooth behavior beyond the interest energy interval $(\varepsilon_1, \varepsilon_2)$ during the Metropolis dynamics.

In order to obtain a caloric curve $\beta$ *versus* $\varepsilon$ with approximately $M$ points with $\langle\varepsilon\rangle$ more or less uniformly distributed in the interval $(\varepsilon_1, \varepsilon_2)$, the canonical parameter $\eta$ can be increased as follows:

$$\eta_{i+1} = \begin{cases} \eta_i + c & \text{if } \langle\varepsilon\rangle > \varepsilon_2, \\ \eta_i \exp\left(\frac{1}{M}\lambda(\varepsilon_2 - \varepsilon_2)\right) & \text{if } \langle\varepsilon\rangle \in (\varepsilon_1, \varepsilon_2), \\ \eta_i + c\exp\left(\lambda(\varepsilon_2 - \varepsilon_1)\right) & \text{otherwise,} \end{cases} \quad (15)$$

where $c > 0$ in the $\beta$ step outside the interest energy interval $(\varepsilon_1, \varepsilon_2)$.

The reader may notice by reexamining the equation (13) that a very large value of the numeric constant $\lambda$ leads to a very small energy dispersion $\delta\varepsilon$, provoking in this way an increasing of the inverse temperature dispersion $\delta\beta$ as a consequence of the uncertainly relation (11). An appropriate prescription of $\lambda$ in order to minimize the dispersion $\left\langle\delta p^2\right\rangle = \left\langle\delta\beta^2 + \delta\varepsilon^2\right\rangle$ in the caloric curve ($\varepsilon$ and $\beta$ in dimensionless units) is given by:

$$\beta_c\lambda \gtrapprox 1. \quad (16)$$

Taking into consideration all the above exposed, microcanonical caloric curve $\beta(\varepsilon) = \partial s(\varepsilon)/\partial\varepsilon$ can be obtained by using our GCMMC methods as follows:

$$\beta\left[\langle\varepsilon\rangle \pm \delta\varepsilon\right] = \eta\left\langle\xi(\varepsilon)\right\rangle \pm \delta\beta, \quad (17)$$

where

$$\delta\beta^2 = \frac{\sigma_\beta^2}{N} \equiv \eta^2\left(\left\langle\xi^2(\varepsilon)\right\rangle - \left\langle\xi(\varepsilon)\right\rangle^2\right), \quad (18)$$

$$\delta\varepsilon^2 = \frac{\sigma_\varepsilon^2}{N} \equiv \left\langle\varepsilon^2\right\rangle - \left\langle\varepsilon\right\rangle^2, \quad (19)$$

while the second derivative of the entropy or curvature $\kappa(\varepsilon) = \partial^2 s(\varepsilon)/\partial\varepsilon^2$ can be given by:

$$\kappa(\langle\varepsilon\rangle) \simeq (\sigma_\varepsilon\sigma_\beta - 1)/\sigma_\varepsilon^2, \quad (20)$$

in accordance with the equation (11). The error $\delta\kappa$ in the curvature after $n$ Metropolis iterations can be estimated by the formula:

$$\delta\kappa \simeq \left\langle 2|\kappa| + 1/\sigma_\varepsilon^2\right\rangle\sqrt{\frac{8\tau}{n}}, \quad (21)$$

where $\tau$ is the decorrelation time, that is, the minimum of Monte Carlo iterations necessary to generate effectively independent, identically distributed samples in the Metropolis dynamics.

## III. A SIMPLE APPLICATION

Let us apply the GCMMC method in order to perform the microcanonical description of a Potts model [10]:

$$H = \sum_{(i,j)}\left\{1 - \delta_{\sigma_i\sigma_j}\right\}, \quad (22)$$

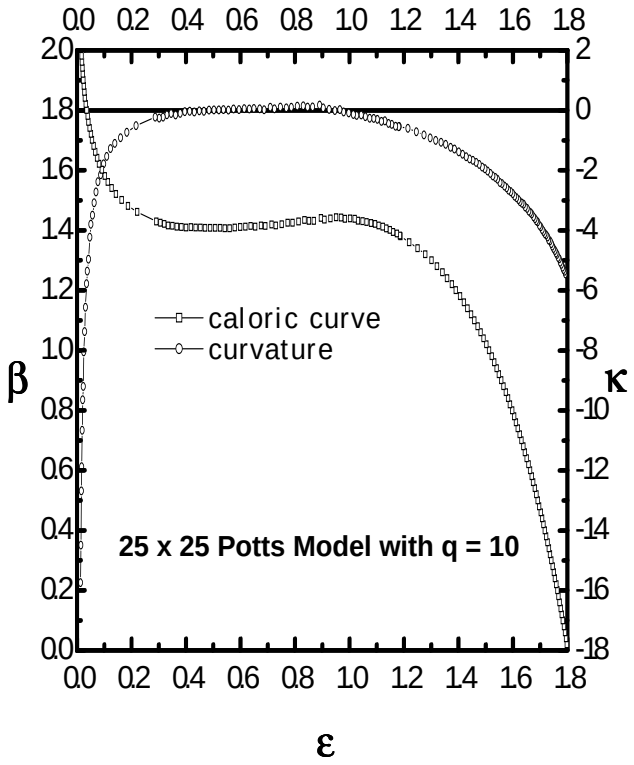


FIG. 1: Microcanonical caloric curve $\beta(\varepsilon) = \partial s(\varepsilon)/\partial\varepsilon$ and curvature $\kappa(\varepsilon) = \partial^2 s(\varepsilon)/\partial\varepsilon^2$ of the $25 \times 25$ Potts model with $q = 10$ states with periodic boundary conditions obtained by using the GCMMC algorithm. Notice the energetic region with a negative heat capacity. Errors are smaller than the symbols linear dimension.

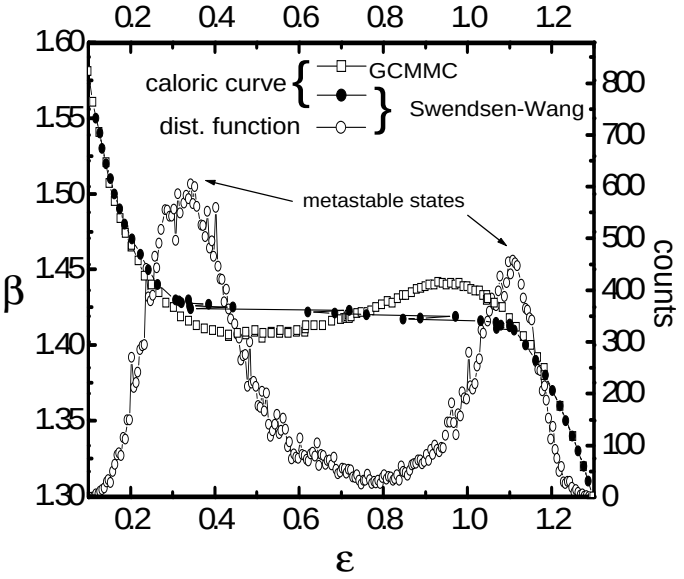


FIG. 2: Comparative study between the GCMMC and the Swendsen-Wang (SW) cluster algorithm. The SW algorithm is unable to describe the microcanonical states with a negative heat capacity. Notice the bimodal character of the energy distribution function at $\beta = 1.42$.

on a two dimensional lattice (here with periodic boundary conditions) of $N = L \times L$ spins with $q = 10$ possible values (components). The sum is over pairs of nearest neighbor lattice points only and $\sigma_i$ is the spin state at the *i-th* lattice point. Generally speaking, this model system admits a ferromagnetic interpretation by introducing the bidimensional vector variables $\mathbf{s}_i = [\cos(\kappa_q \sigma_i), \sin(\kappa_q \sigma_i)]$ with $\kappa_q = 2\pi/q$, and defining the total magnetization as follows $\mathbf{M} = \sum_i \mathbf{s}_i$.

As elsewhere shown, the $q = 10$ states Potts model exhibits a first-order phase transition associated to the ensemble inequivalence, which provokes the existence of a supercritical slowing down during the ordinary Metropolis dynamics based on the consideration of the Gibbs canonical ensemble. Clusters algorithms, like Swendsen-Wang or Wolf algorithms [11], do not help in this case [12] due to they are still based on the consideration of the canonical ensemble, and consequently, the supercritical slowing down associated to the ensemble inequivalence persists [13].

This difficulty is successfully overcome by using the Multicanonical Monte Carlo method [6, 7], which reduces the exponential divergence of the correlation times with respect to system size to a power at the first-order phase transitions [14]. Multicanonical ensemble flattens out the energy distribution, which allows the computation of the density of states $\Omega(E, N)$ for all values of $E$ in only one run. This feature of the Multicanonical ensemble becomes a disadvantage when we are also interested in the direct computation of the microcanonical average of other microscopic observables at a given value of the energy, i.e. the magnetization density dependence $\mathbf{m}(\varepsilon) = \langle \mathbf{M} \rangle / N$ of the Potts model (22) with $q = 10$. This aim can be easily performed by using the GCMMC algorithm.

A preliminary calculation by using the MMC allows us to set the interest energetic window with $\varepsilon_1 = 0.2$ and $\varepsilon_2 = 1.2$ in which takes place the critical slowing down associated with the existence of a first-order phase transition in this model for $L = 25$. The inverse critical temperature was estimated as $\beta_c \simeq 1.4$, allowing us to set $\lambda = 0.8$. Besides, we also set $M = 50$ and $c = 0.02$ in the $\eta$ increasing given by the equation (15). The caloric $\beta(\varepsilon)$ and curvature $\kappa(\varepsilon)$ curves obtained by using the GCMMC algorithm with $n = 10^5$ Metropolis iterations for each point is shown in the FIG.1. A comparative study between the present method and the Swendsen-Wang clusters algorithm [13] is shown in the FIG.2.

The backbending in the caloric curve $\beta$ *versus* $\varepsilon$ is directly associated to the existence of a negative heat capacity $c(\varepsilon) = -\beta^2(\varepsilon)/\kappa(\varepsilon)$ when $\varepsilon \in (\varepsilon_a, \varepsilon_b)$ with $\varepsilon_a = 0.51$ and $\varepsilon_b = 0.93$, which is a feature of a first-order phase transition in a small system becoming extensive in the thermodynamic limit. Since the heat capacity is always positive within the canonical ensemble,

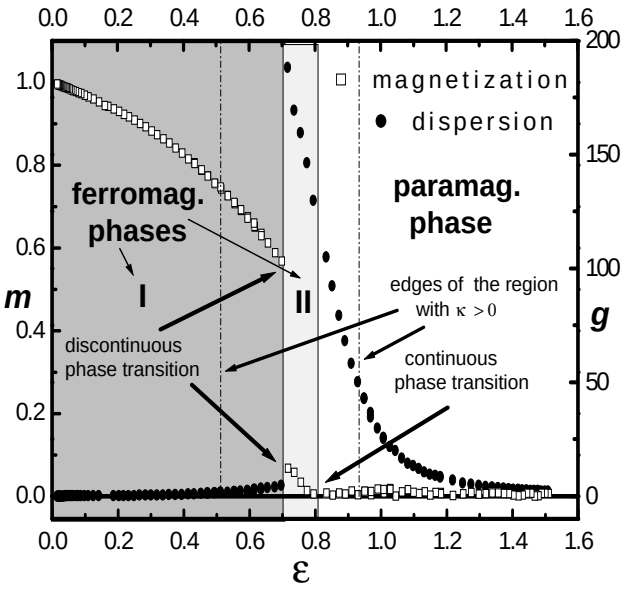


FIG. 3: Magnetic properties of the model within the microcanonical ensemble in which is shown the existence of two phase transitions at $\varepsilon_{ff} \simeq 0.7$ (ferro-ferro) and $\varepsilon_{fp} \simeq 0.8$ (ferro-para).

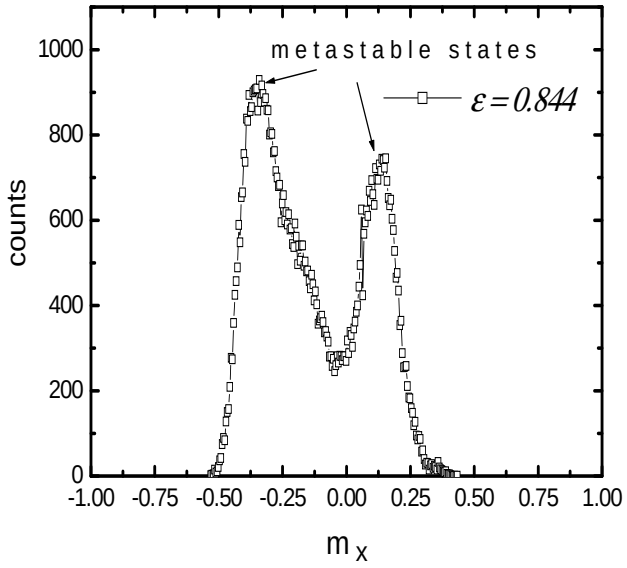


FIG. 4: Histogram of the projection of the microscopic magnetization along the direction of the spontaneous magnetization of the ferromanet type I, which demostrates the existence of metastable states when $\varepsilon = 0.844$.

$c_c = N\beta^2 \left\langle \Delta\varepsilon^2 \right\rangle_c \geq 0$, such anomalous regions are inaccessible in this description ($\langle \cdots \rangle_c$ denotes the canonical average). This fact evidences the existence of a significant *lost of information* about the thermodynamical features of the system during the occurrence of a first-order phase transitions when the canonical ensemble is used instead of the microcanonical one. This difficulty is successfully overcome by the GCMMC algorithm, which is able to predict the microcanonical average of the microscopic observables in these anomalous regions where any others Monte Carlo methods based on the consideration of the Gibbs canonical ensemble such as the original MMC, the Swendsen-Wang and the Wolff single cluster algorithms certainly do not work.

This fact is clearly illustrated in the FIG.2, which evidences that the Swendsen-Wang algorithm is unable to describe the thermodynamic states with a negative heat capacity: its results within the anomalous region differ significantly from the ones obtained by using the GCMMC algorithm. The Swendsen-Wang dynamics exhibits here an erratic behavior originated from the competition of the two metastable states present in the neighborhood of the critical point (the energy distribution function in the canonical ensemble is bimodal when $\beta \in (\beta_1, \beta_2)$, where $\beta_1 = 1.405$ and $\beta_2 = 1.445$, being this feature the origin of the supercritical slowing down).

As already shown by Gross in ref.[15], a negative heat capacity in a system with short-range interactions can be associated to the existence of a non-vanishing interphase surface tension. Other quantities like the transition temperature $\beta_{cr}$ and the latent heat $q_{lat}$ can be derived easily from the caloric curve $\beta(\varepsilon)$. Following the same procedure developed by Gross, our calculations allow us to obtain the following estimates for the $q = 10$ states Potts model with $L = 25$: $\beta_{cr} \simeq 1.421$ and $q_{lat} \simeq 0.78$.

The study of the magnetic properties of this model within the microcanonical ensemble illustrated in the FIG.3, shows us that the existence of the non-vanishing interphase surface tension is not the only one information hidden behind of a negative heat capacity within the canonical description. The modulus of the magnetization density $m(\varepsilon)$ evidences what could be considered as the signature of two *phase transitions within the microcanonical description of this model system*: a continuous (paramagnetic-ferromagnetic) phase transition at the critical point $\varepsilon_{fp} \simeq 0.8$, and a discontinuous (ferro-ferro) phase transition at $\varepsilon_{ff} \simeq 0.7$ (from a low magnetized ferromagnetic type II phase towards a high magnetized ferromagnetic type I one). The investigation of these interesting behaviors deserves a further study.

Most of thermodynamic points of this dependences were obtained from a data of $n = 10^5$ Metropolis iterations, with the exception of all those points belonging to the energetic interval $(0.7, 0.93)$ where very large fluctuations of the magnetization density were observed. The possibility of the GCMMC algorithm of performing a localized computation of the microcanonical averages at a given value of the energy allows us to increase the Metropolis iterations $n$ up to $5 \times 10^6$ for each point within the above energetic range in order to reduce the significant dispersion of the expectation values observed there.

The very large fluctuations, the peculiar behavior of the dispersion $g(\varepsilon) = \left\langle (\mathbf{M} - \langle \mathbf{M} \rangle)^2 \right\rangle / N$, the qualitative form of the magnetization curve $m(\varepsilon)$ shown in FIG.3,

as well as the apparent large relaxation times of the expectation values during the GCMMC dynamics, suggest us the presence of several metastable states with different magnetization densities at a given energy within this last region, whose existence is shown in the FIG.4.

The anomalies observed in the thermodynamic characterization of the $q = 10$ state Potts model suggest strongly the existence of the critical slowing down phenomena within the "microcanonical description" provided by the GCMMC algorithm. This fact inspires the development of nonlocal Monte Carlo algorithms based on the consideration of the generalized canonical ensemble (1) in order to address the microcanonical description of more larger systems undergoing a discontinuous (first-order) phase transitions within the canonical description.

## IV. CONCLUSIONS

We have presented a very simple methodology for improving the ordinary Metropolis importance sampling algorithm [8] in order to allow the computation of the microcanonical averages during the occurrence of the first-order phase transitions in systems with short-range interactions. The key of our approach is the consideration of certain generalized canonical ensemble (1) inspired on the reparametrization invariance of the microcanonical description [9], which becomes equivalent to the microcanonical ensemble when the size $N$ of the interest system is large enough.

A direct advantage of this new methodology is the possibility of performing a localized computation of the any microcanonical average at a given value of the energy, and avoid in this way the unnecessary computation of the whole energy range, a feature of many other Monte Carlo technics based on reweighting the energy histogram [16, 17, 18]. The existence of anomalies within the microcanonical description of the $q = 10$ states Poots model inspires the further development of nonlocal Monte Carlo algorithms based on the consideration of the generalized canonical ensemble (1).


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